ACCURACY AND CALIBRATION OF HIGH EXPLOSIVE THERMODYNAMIC EQUATIONS OF STATE

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14. ABSTRACT

   The Jones-Wilkins-Lee-Baker (JWLB) equation of state was developed to more accurately describe overdriven detonation, while maintaining an accurate description of high explosive products expansion work output. The increased mathematical complexity of the JWLB high explosive equations of state provides increased accuracy for practical problems of interest. Increased numbers of parameters is often justified based on improved physics descriptions, but can also mean increased calibration complexity. A generalized extent of aluminum reaction, the Jones-Wilkins-Lee (JWL) based equation of state was developed in order to more accurately describe the observed behavior of aluminized explosives detonation products expansion. A calibration method was developed to describe the un-reacted, partially reacted, and completely reacted explosive using non-linear optimization. A reasonable calibration of a generalized extent of aluminum reaction, JWLB equation of state as a function of aluminum reaction fraction has not yet been achieved due to the increased mathematical complexity of the JWLB form.

15. SUBJECT TERMS
Jones-Wilkins-Lee-Baker (JWLB), JWLB based equation of state, Aluminized explosives detonation products expansion, Non-linear optimization

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INTRODUCTION

Increased mathematical complexity of high explosive equations of state does not guarantee increased accuracy for practical problems of interest. Increased numbers of parameters is often justified based on improved physics descriptions, but can also mean increased calibration complexity. This issue is discussed in relationship to the Jones-Wilkins-Lee-Baker (JWLB) thermodynamic equation of state and a newly developed generalized extent of aluminum reaction Jones-Wilkins-Lee (JWL) based equation of state. The JWLB thermo-dynamic equation of state was developed to more accurately describe overdriven detonation, while maintaining an accurate description of high explosive products expansion work output (ref. 1). The equation of state is more mathematically complex than the JWL equation of state, as it includes an increased number of parameters to describe the principle isentrope, as well as a Gruneisen parameter formulation that is a function of specific volume. The JWLB mathematical form is:

$$P = \sum_n A_i \left(1 - \frac{\omega}{R_i V^*} \right) e^{-R_i V^*} + \frac{\lambda E}{V^*} \tag{1}$$

$$\lambda = \sum_i (A_{\lambda i} V^* + B_{\lambda i}) e^{-R \lambda i V^*} + \omega \tag{2}$$

where V^* is the relative volume, E is the product of the initial density and specific internal energy and λ is the Gruneisen parameter. Often it is questioned whether the increased mathematical complexity over JWL is of value, as increased numbers of parameters can mean increased calibration complexity and does not guarantee increased accuracy for practical problems of interest. Two methods of parameter calibration have been used to date: empirical calibration to cylinder test data and formal optimization using JAGUAR thermochemical predictions. This paper will only discuss the formal optimization using JAGUAR thermochemical predictions (ref. 2).

ANALYTIC CYLINDER MODEL

An analytic cylinder test model that uses JWL or JWLB equations of state was developed, which provides excellent agreement with high rate continuum modeling (ref. 3). Isentropic expansion is assumed for the expanding detonation products from the Chapman-Jouguet state. In addition, constant detonation products are assumed across spherical surfaces that perpendicularly intersect the cylinder inside wall. The products mass velocities are assumed perpendicular to the spherical surfaces. These assumptions - along with mass, momentum, and energy conservation - result in the final model. Figure 1 presents a sketch representation of the analytic cylinder test model.
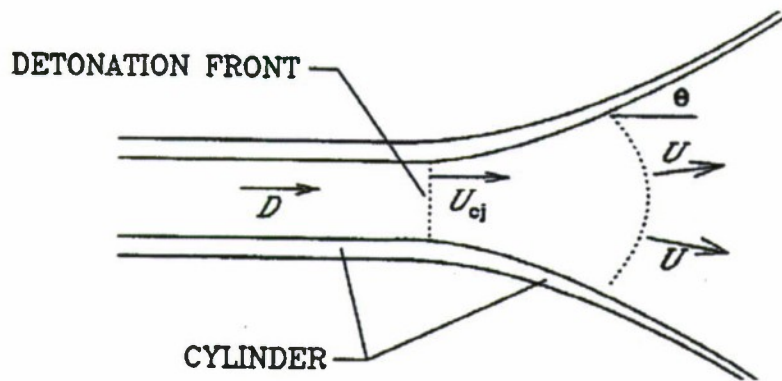
Figure 1
Analytic cylinder test model

JONES-WILKINS-LEE-BAKER EQUATION OF STATE

One method of JWLB parameterization is to directly fit the predicted pressure and Gruneisen parameter versus specific volume behaviors predicted by JAGUAR. Formal non-linear optimization is used for the parameterization procedure. The example presented is using the high energy explosive LX-14. The LX-14 JWL and JWLB equation of states were parameterized using the JAGUAR predictions and non-linear optimization routines. The resulting JWL and JWLB equations of state were then used to model a standard 25-mm outside and 20-mm inside cylinder test and compare to experimental data using the analytic cylinder test model and the high rate continuum model CALE (ref. 4). Table 1 and figure 2 present the resulting outside cylinder velocity results at different inside cylinder cross-sectional areas. The results clearly show the improved agreement to experimental data obtained when using the more mathematically complex JWLB mathematical form. The improved agreement is attributed to the improved agreement to the JAGUAR predicted detonation products behavior that is achieved using the JWLB form.

Table 1
LX-14 JWL and JWLB cylinder test velocity predictions (km/s) compared to experimental data

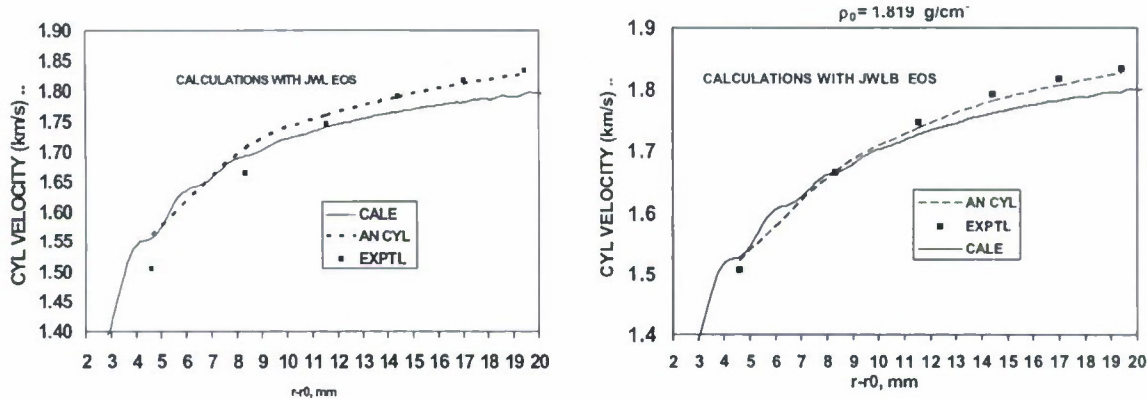| A/AO	AVG EXPTL	ANALYTIC CYLINDER		CALE	
		JWL	JWLB	JWL	JWLB
2	1.505	1.562	1.519	1.555	1.527
3	1.664	1.705	1.667	1.692	1.665
4	1.745	1.759	1.738	1.74	1.727
5	1.791	1.79	1.78	1.765	1.761
6	1.817	1.812	1.807	1.781	1.782
		ABS % ERROR			
2		3.787	0.930	3.322	1.462
3		2.464	0.180	1.683	0.060
4		0.802	0.401	0.287	1.032
5		0.056	0.614	1.452	1.675
6		0.275	0.550	1.981	1.926
7		0.273	0.382	2.073	1.946

Figure 2
LX-14 JWL and JWLB cylinder test predictions compared to experiments

EIGENVALUE DETONATION

Previous studies have shown that the traditional Chapman-Jouguet detonation theory does not explain the observed detonation states and expansion behavior achieved by aluminized explosives. The detonation behavior of these explosives has been studied using both experimental data and JAGUAR thermochemical calculations. In order to account for the observed behavior of the aluminized explosives investigated, a model was postulated in which the explosive expands through a reaction zone at a detonation velocity often controlled by the Hugoniot for zero aluminum reaction (refs. 5 and 6). At the zero aluminum reaction Hugoniot, the aluminum is unreacted while the other gaseous and solid C-H-N-O products are in equilibrium. For the partially reacted aluminum Hugoniots, the reacted aluminum fraction detonation product (aluminum oxide) is in equilibrium with the other C-H-N-O products. For the reaction zone, the necessary Hugoniot and Rayleigh line relationships must be satisfied. However, for the aluminized explosives investigated to date, the unreacted aluminum Hugoniot curves actually fall above the reacted aluminum Hugoniots in P-V space. Therefore, the minimum detonation velocity solution occurs with the Raleigh line intersecting the zero aluminum reaction Hugoniot at the tangency point. The associated eigenvalue detonation velocity is the velocity that would be measured experimentally. Two associated thermodynamic equations of state representations were developed. For relatively fast aluminum reaction, an eigenvalue JWLB equation of state and calibration methodology was developed. The resulting eigenvalue JWLB equation of state is more accurate at early detonation products expansion compared to an eigenvalue JWL equation of state. For a relatively slower aluminum reaction rate, a partial reaction JWL thermodynamic equation of state and calibration method was developed to describe the unreacted, partially reacted, and completely reacted explosive.

EIGENVALUE JWLB EQUATION OF STATE

The same JWLB parameterization was used to directly fit the predicted pressure and Gruneisen parameter versus specific volume behaviors predicted by JAGUAR. The examples presented used the new aluminized combined effects explosives PAX-30 and PAX-29. PAX-30 and PAX-29 are 15% by weight aluminum based on HMX and CL-20, respectively. As the PAX-30 and PAX-29 explosives produce eigenvalue, rather than traditional Chapman-Jouguet detonations, a modified analytic cylinder test model was developed that assumes isentropic

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expansion from the eigenvalue detonation produced weak point [WPT (ref. 7)]. Table 2 and figure 3 present the resulting outside cylinder velocity results at different inside cylinder cross-sectional areas for PAX-30. Table 3 and figure 4 present the results for PAX-29. The results clearly show the improved agreement to experimental data obtained when using the more mathematically complex JWLB mathematical form. Again, the improved agreement is attributed to the improved agreement to the JAGUAR predicted detonation products behavior that is achieved using the JWLB form.

Table 2
PAX-30 JWL and JWLB cylinder test predictions compared to experiments

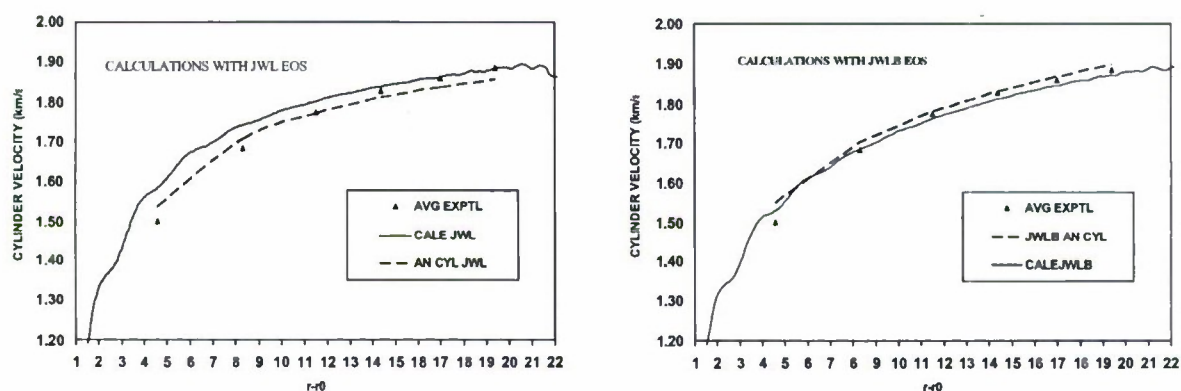| A/A0		ANALYTIC CYLINDER			CALE	
	AVG EXPTL	JWL	JWLB	JWLB WPT	JWL	JWLB
2	1.499	1.599	1.55	1.541	1.582	1.531
3	1.682	1.759	1.702	1.703	1.741	1.685
4	1.774	1.823	1.780	1.779	1.801	1.762
5	1.827	1.862	1.831	1.825	1.837	1.811
6	1.859	1.89	1.868	1.856	1.862	1.845
7	1.883	1.911	1.897	1.879	1.883	1.872
			ABS % ERROR			
2		6.6711	3.4023	2.8019	5.5370	2.135
3		4.5779	1.1891	1.2485	3.5077	0.178
4		2.7621	0.3157	0.2818	1.5220	0.676
5		1.9157	0.2189	0.1095	0.5473	0.876
6		1.6676	0.4841	0.1614	0.1614	0.753
7		1.4870	0.7435	0.2124	0.0000	0.584
AVG ERROR		**3.1802**	**1.0589**	**0.8026**	**1.8792**	**0.867**

Figure 3
PAX-30 JWL and JWLB cylinder test predictions compared to experiments

Table 3
PAX-29 JWL and JWLB cylinder test predictions compared to experiments

| A*	AVG EXPTL	ANALYTIC CYLINDER			CALE	
		JWL	JWLB	JWLB WPT	JWL	JWLB
2	1.601	1.678	1.636	1.617	1.663	1.614
3	1.777	1.843	1.792	1.781	1.822	1.772
4	1.868	1.908	1.869	1.859	1.883	1.844
5	1.919	1.948	1.92	1.907	1.922	1.896
6	1.950	1.976	1.957	1.941	1.947	1.93
7	1.970	1.998	1.985	1.965	1.966	1.957
		ABS % ERROR				
2		4.809	2.186	0.999	3.873	0.812
3		3.714	0.844	0.225	2.532	0.281
4		2.141	0.054	0.482	0.803	1.285
5		1.511	0.052	0.625	0.156	1.199
6		1.333	0.359	0.462	0.154	1.026
7		1.421	0.761	0.254	0.203	0.660
AVG ERROR		**2.488**	**0.709**	**0.508**	**1.287**	**0.877**
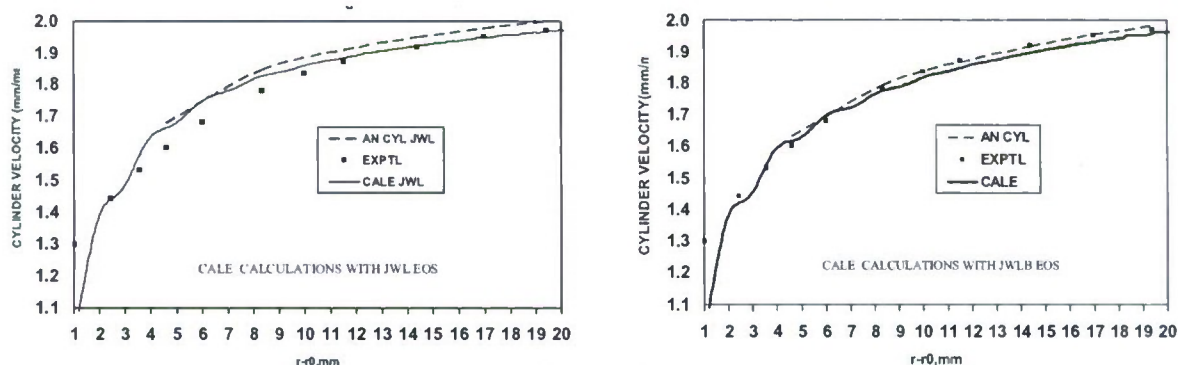
Figure 4
PAX-29 JWL and JWLB cylinder test predictions compared to experiments.

GENERALIZED JWLB EQUATION OF STATE

In order to aid in the effective determination and representation of the behavior of aluminized explosives with a slower aluminum reaction, a calibration optimization procedure was developed to obtain relationships for the variation of JWL constants with reaction fraction of aluminum, X. This new thermodynamic equation of state is parameterized using the JAGUAR thermochemical potential computer program (ref. 8). This *P-V-E* equation of state has the advantage for continuum modeling that it is parameterized directly using partially reacted states, rather than balanced between unreacted and fully reacted equation of states. This parameterization methodology insures that the *P-V-E* behavior of the partially reacted materials equation of state agrees appropriately (and precisely) for Hugoniot and isentropes. The partial reaction JWL equation of state is

$$P = \sum_{1}^{2} A_i \left(1 - \frac{\omega}{R_i V^*} \right) e^{-R_i V^*} + \frac{\omega E}{V^*} \tag{3}$$

where $V*$ is the relative volume and E is the product of the initial density and specific internal energy. The constants A_i and R_i of equation 3 are assumed to vary linearly with fraction aluminum reaction as

$$A_i = a_{i1} + a_{i2}X \quad (4)$$

$$R_i = r_{i1} + r_{i2}X \quad (5)$$

In order to find the eight optimum parameters $a_{i1}, a_{i2}, r_{i1}, r_{i2}$ of equations 4 and 5, the objective function is to minimize the sum of the squares of the deviations between pressures calculated with equation 3 and the JAGUAR pressures for the isentropes at 0%, 50%, and 100% aluminum reaction. The eigenvalue detonation velocity and weak point detonation pressure are constrained to be equal to the JAGUAR predicted values. Resulting parameter sets are presented in table 4.

Table 4
Parameters of generalized JWL relationships for aluminized explosives

	PAX-3	PAX-29	PAX-30	PAX-42
	HMX	CL-20	HMX	RDX
Al (wt%)	18	15	15	15
$\rho 0$ (g/cm^3)	1.866	1.999	1.909	1.834
a_{11} (Mbar)	9.5342	15.9932	9.6294	9.9872
a_{12} (Mbar)	6.6006	14.8808	-0.63196	4.9768
a_{21} (Mbar)	0.22167	0.46824	0.10453	0.27971
a_{22} (Mbar)	0.35652	0.50294	0.11400	0.33391
r_{11}	5.0215	5.5721	4.7231	5.1757
r_{12}	1.7141	2.0922	0.33447	1.4267
r_{21}	1.52630	1.74214	1.07379	1.5569
rR_{22}	0.24991	0.24618	0.16594	0.25709
C_1 (Mbar)	7.6510E-3	9.5806R-3	8.2921E-3	8.7711E-3
C_2 (Mbar)	5.8150E-3	5.0455E-3	5.2828E-3	5.2673E-3
W_1	0.5802	0.3407	0.30711	0.31326
W_2	-6.8399E-2	-9.7833E-2	-7.2446E-2	-7.2722E-2

Calculations using the partial reaction JWL equation of state were used to accurately reproduce observed cylinder test data of several aluminized explosives. One of the initial kinetic models considered for the aluminum reaction behavior of the zones is a pseudo first-order model

$$X = 1 - \exp(-DEC(t - t_0)) \quad (6)$$

Figure 5 presents a comparison of experimental and computational cylinder velocities for two 85% HMX and 15% Al by weight compositions with different aluminum particle sizes (refs. 9 and 10].
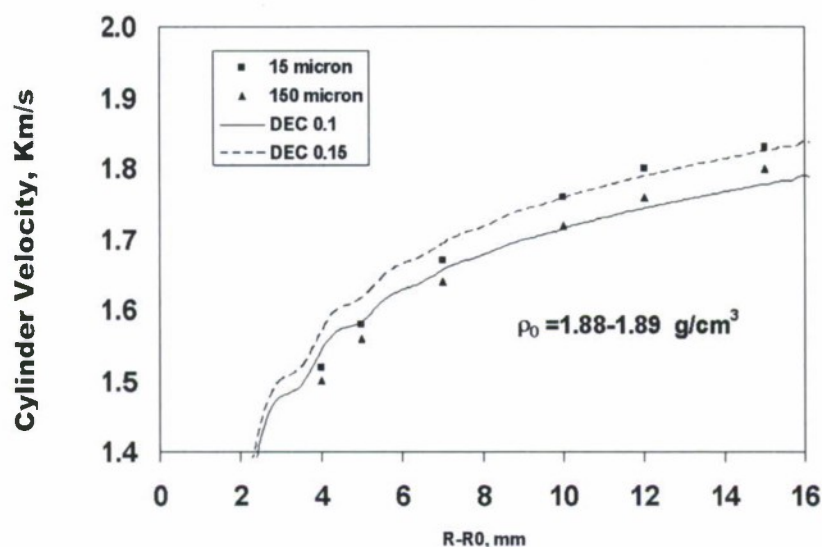
Figure 5
Experiment and modeling comparisons for HMX/Al 85/15

Although the JWLB equation of state provides a more accurate prediction of the early products expansion, a reasonable calibration of the JWLB parameters as a function of aluminum reaction fraction has not yet been achieved due to the mathematical complexity of the JWLB form.

CONCLUSIONS

The results clearly show that the Jones-Wilkins-Lee-Baker (JWLB) equation of state produces improved accuracy for overdriven detonation, while maintaining or increasing the prediction accuracy of the detonation products expansion work output. However, for many practical applications when overdriven detonation or early products expansion phenomenon are not important, the JWL equation of state provides adequate accuracy. The generalized JWL equation of state as a function of aluminum reaction fraction that was developed for slower aluminum reactions was shown to provide improved modeling capability and increased insight for some aluminized explosive compositions. Although the JWLB equation of state provides a more accurate prediction of the early products expansion, a reasonable calibration of the JWLB parameters as a function of aluminum reaction fraction has not yet been achieved due to the mathematical complexity of the JWLB form. Implementations of the JWLB thermodynamic equations of state were completed in the DYNA, CALE, CTH, and ALE-3D hydrocode applications. These thermodynamic equations of state are enabling the improved continuum modeling of overdriven detonation, early detonation products expansion, and aluminized explosives.

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